2-Nitropropane
79-46-9 | DTXSID6020981

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 5.43 days

Global applicability domain: Outside

Local applicability domain index: 3.14e-01

Confidence level: 8.21e-01

Nearest Neighbors from the Training Set

Image not found
Pentane
Measured: 40.7
Predicted: 6.52

Image not found
n-Hexane
Measured: 157
Predicted: 7.45

Image not found
2-Methylhexane
Measured: 12.5
Predicted: 5.54

Image not found
2-Methyloctane
Measured: 40.7
Predicted: 4.23

Image not found
Heptane
Measured: 88.3
Predicted: 7.54